OT-Flow: Optimal Transport for Continuous Normalizing Flows

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Motivation

Continuous Normalizing Flows

A normalizing flow [1] is an invertible mapping $f\colon \mathbb{R}^d \to \mathbb{R}^d$ between an arbitrary probability distribution and a standard normal distribution whose densities we denote by ρ_0 and ρ_1, respectively.

By change of variables, the flow must approximately satisfy

$$\log \rho_0(\boldsymbol{x}) = \log \rho_1(f(\boldsymbol{x})) + \log|\det \nabla f(\boldsymbol{x})| \quad \text{for all} \quad \boldsymbol{x} \in \mathbb{R}^d. \qquad (1)$$

In continuous normalizing flows (CNFs), f is obtained by solving the neural ordinary differential equation (ODE) [2, 3]

$$\partial_t \begin{bmatrix} \boldsymbol{z}(\boldsymbol{x},t) \\ \ell(\boldsymbol{x},t) \end{bmatrix} = \begin{bmatrix} \mathbf{v}(\boldsymbol{z}(\boldsymbol{x},t),t;\boldsymbol{\theta}) \\ \mathrm{tr}\left(\nabla \mathbf{v}(\boldsymbol{z}(\boldsymbol{x},t),t;\boldsymbol{\theta})\right) \end{bmatrix}, \quad \begin{bmatrix} \boldsymbol{z}(\boldsymbol{x},0) \\ \ell(\boldsymbol{x},0) \end{bmatrix} = \begin{bmatrix} \boldsymbol{x} \\ 0 \end{bmatrix}, \qquad (2)$$

where, for artificial time $t \in [0,T]$,

- $\boldsymbol{x}$ maps to $f(\boldsymbol{x}) = \boldsymbol{z}(\boldsymbol{x},T)$ following trajectory $\boldsymbol{z}\colon \mathbb{R}^d \times [0,T] \to \mathbb{R}^d$
- dynamics are modeled by neural network layer $\mathbf{v}\colon \mathbb{R}^d \times [0,T] \to \mathbb{R}^d$ parameterized by weights $\boldsymbol{\theta}$
- $\ell(\boldsymbol{x},T) = \log\det \nabla f(\boldsymbol{x})$, derived from Jacobi's Formula [2]

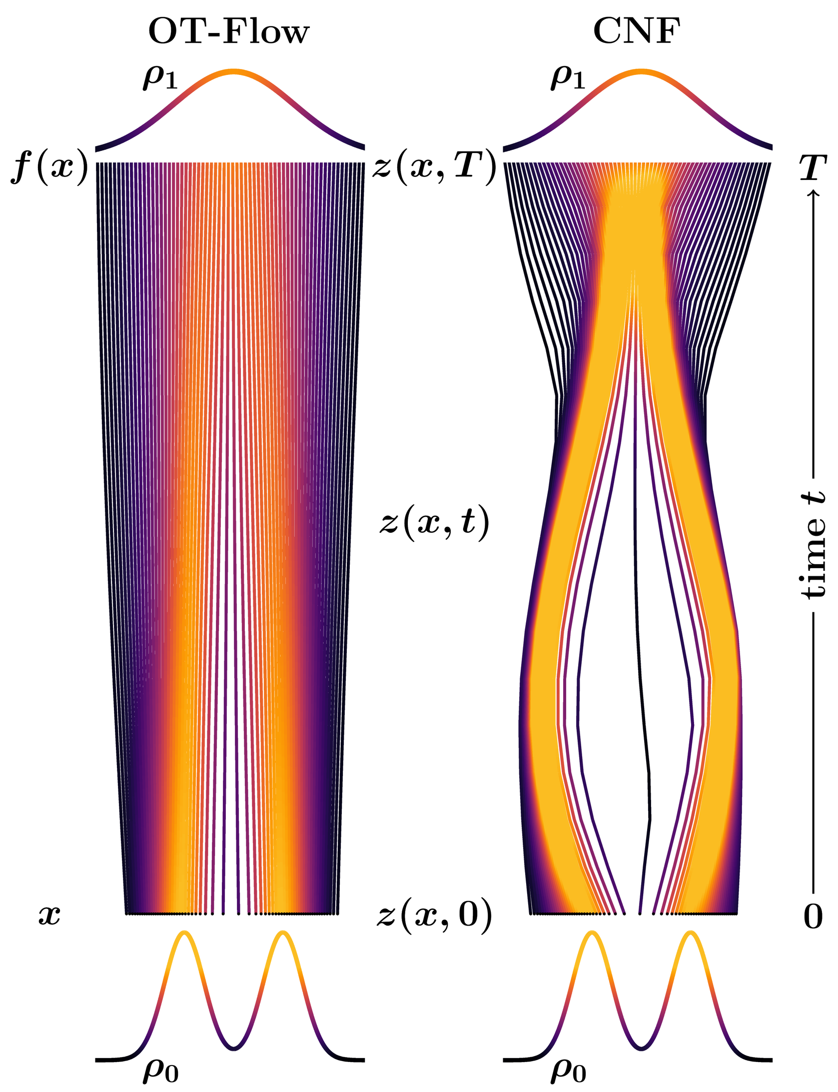


Figure 1: While a CNF can have curved trajectories, OT-Flow's are straight (modification of Fig. 1 in [3, 4]).

Microscale: an arbitrary sample $\boldsymbol{x}$ maps to a normally distributed $f(\boldsymbol{x})$
Macroscale: ρ_0 maps to ρ_1

CNFs are trained by solving the optimization problem [1, 3]

$$\min_{\boldsymbol{\theta}} \ \mathbb{E}_{\rho_0(\boldsymbol{x})} \left\{ C(\boldsymbol{x},T) := \frac{1}{2}\|\boldsymbol{z}(\boldsymbol{x},T)\|^2 - \ell(\boldsymbol{x},T) + \frac{d}{2}\log(2\pi) \right\} \quad \text{s.t.} \quad (2). \qquad (3)$$

High Training Costs

- Many functions evaluations are needed to solve (2)
- Using automatic differentiation (AD) to compute the trace requires separate matrix-vector products with the Jacobian and all d standard basis vectors, costing $\mathcal{O}(d^2)$ FLOPs in total

Our Contributions

Optimal Transport (OT) Incorporating OT, we regularize the CNF so it has a unique solution (Figure 1).

Analytic Exact Trace We derive formulae for an exact trace computation with complexity $\mathcal{O}(d)$ FLOPs.

Optimal Transport

L_2 Transport Costs Add transport costs

$$L(\boldsymbol{x},T) = \int_0^T \frac{1}{2}\|\mathbf{v}(\boldsymbol{z}(\boldsymbol{x},t),t)\|^2 \, \mathrm{d}t. \qquad (4)$$

to (3) to penalize the arc-length of the trajectories.

Potential Function By the Pontryagin maximum principle [5], there exists a scalar potential function $\Phi\colon \mathbb{R}^d \times [0,T] \to \mathbb{R}$ such that

$$\mathbf{v}(\boldsymbol{x},t;\boldsymbol{\theta}) = -\nabla\Phi(\boldsymbol{x},t;\boldsymbol{\theta}).$$

Idea: Analogous to classical physics, samples move to minimize their potential
⇒ We parameterize potential Φ instead of $\mathbf{v}$.

HJB Regularizer At optimality, Φ satisfies the Hamilton-Jacobi-Bellman (HJB) equation [6]

$$-\partial_t \Phi(\boldsymbol{x},t) + \frac{1}{2}\|\nabla\Phi(\boldsymbol{z}(\boldsymbol{x},t),t)\|^2 = 0,$$
$$\Phi(\boldsymbol{x},T) = G(\boldsymbol{x})$$

where

$$G(\boldsymbol{z}(\boldsymbol{x},T)) = 1 + \log\left(\rho_0(\boldsymbol{x})\right) - \log\left(\rho_1(\boldsymbol{z}(\boldsymbol{x},T))\right) - \ell(\boldsymbol{x},T)$$

To penalize sub-optimality, use HJB regularizer

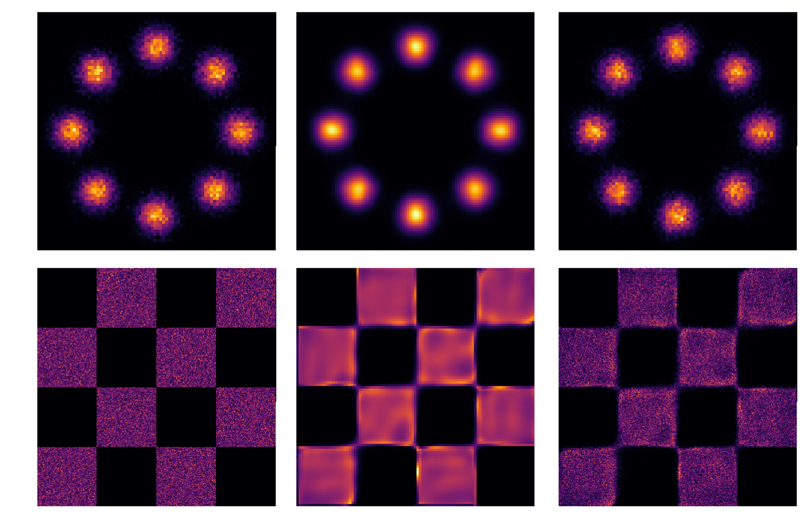
$$R(\boldsymbol{x},T) = \int_0^T \left| \partial_t\Phi(\boldsymbol{z}(\boldsymbol{x},t),t) - \frac{1}{2}\|\nabla\Phi(\boldsymbol{z}(\boldsymbol{x},t),t)\|^2 \right| \mathrm{d}t \qquad (5)$$

OT-Flow Optimization Problem

$$\min_{\boldsymbol{\theta}} \ \mathbb{E}_{\rho_0(\boldsymbol{x})} \left\{ C(\boldsymbol{x},T) + L(\boldsymbol{x},T) + R(\boldsymbol{x},T) \right\} \ \text{s.t. (2), (4), (5)}$$

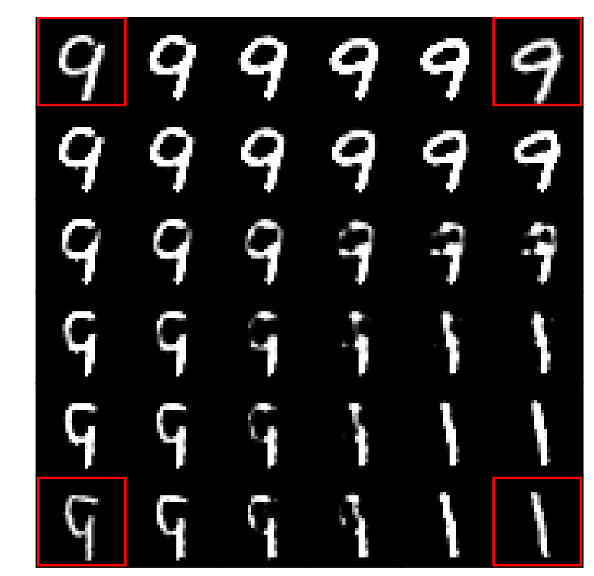
Results

Two-dimensional Toy Density Estimation



19x speedup in training and 28x speedup in inference relative to the state-of-the-art FFJORD [3] on five real datasets of dimensionality $d = 6, 8, 21, 43, 63$

MNIST Synthetic Generation



Encoder $B\colon \mathbb{R}^{784} \to \mathbb{R}^{128}$,
Decoder $D\colon \mathbb{R}^{128} \to \mathbb{R}^{784}$
such that $D(B(\boldsymbol{x})) \approx \boldsymbol{x}$

Train OT-Flow mapping samples $B(\boldsymbol{x})$ to $\mathcal{N}(0, \boldsymbol{I}_{128})$

For two MNIST images $\boldsymbol{x}_1, \boldsymbol{x}_2 \in \mathbb{R}^{784}$, interpolate in the latent space to create synthetic image

$$\boldsymbol{y}(\lambda) = D(f^{-1}(\lambda f(B(\boldsymbol{x}_1)) + (1-\lambda) f(B(\boldsymbol{x}_2)))).$$

Original images are boxed in red.

Links

Corresponding Paper Preprint:

arxiv.org/abs/2006.00104

PyTorch implementation is available on Emory's Machine Learning and Inverse Problems repository:

github.com/EmoryMLIP/OT-Flow

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References

[1] D Rezende and S Mohamed *Variational Inference with Normalizing Flows.* ICML, 2015.

[2] Chen et al. *Neural Ordinary Differential Equations.* NeurIPS, 2018.

[3] W Grathwohl et al. *FFJORD: Free-form continuous dynamics for scalable reversible generative models.* ICLR, 2019.

[4] C Finlay et al. *How to train your neural ODE.* arXiv:2002.02798, 2020.

[5] L Evans *An Introduction to Mathematical Optimal Control Theory Version 0.2.* 2013.

[6] L Evans *Partial differential equations and Monge-Kantorovich mass transfer.* Current developments in mathematics, 1997.

Exact Trace

Exploit $\mathrm{tr}\left(\nabla^2\Phi(\boldsymbol{s};\boldsymbol{\theta})\right) = \mathrm{tr}\left(\boldsymbol{E}^\top \nabla^2_{\boldsymbol{s}}\Phi(\boldsymbol{s};\boldsymbol{\theta})\,\boldsymbol{E}\right)$ for $\boldsymbol{E} =$ `eye(d+1,d)`. Details in Links.

In runtime, exact trace is competitive with estimators used in other CNFs.